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J. Math. Anal. Appl. 288 (2003) 28–46

Journal of MATHEMATICAL ANALYSIS AND APPLICATIONS

www.elsevier.com/locate/jmaa

The numerical approximation of center manifolds in Hamiltonian systems

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Received 17 October 2002

Submitted by W.L. Wendland

Abstract

In this paper we develop a numerical method for computing higher order local approximations of center manifolds near steady states in Hamiltonian systems. The underlying system is assumed to be large in the sense that a large sparse Jacobian at the equilibrium occurs, for which only a linear solver and a low-dimensional invariant subspace is available. Our method combines this restriction from linear algebra with the requirement that the center manifold is parametrized by a symplectic mapping and that the reduced equation preserves the Hamiltonian form. Our approach can be considered as a special adaptation of a general method from Numer. Math. 80 (1998) 1–38 to the Hamiltonian case such that approximations of the reduced Hamiltonian are obtained simultaneously. As an application we treat a finite difference system for an elliptic problem on an infinite strip.

Keywords: Center manifolds; Hamiltonian systems; Numerical methods; Bordered linear systems

1. Introduction

We consider a Hamiltonian system of the form

$$\dot{x} = J\nabla H(x), \quad x \in \mathbb{R}^{2n}, \tag{1.1}$$

where J is an invertible skew symmetric matrix.

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1 Supported by the Volkswagen Foundation of Germany in 1999–2002.
2 Supported by DFG Research group ‘Spectral analysis, asymptotic distributions and stochastic dynamics.’

0022-247X/$ – see front matter
doi:10.1016/j.jmaa.2003.05.001

It is assumed that $x = 0$ is an equilibrium point of (1.1), i.e.,

$$\nabla H(0) = 0$$

and that the Hamiltonian matrix $A = JH^0_{xx}$ has $2l$ eigenvalues on the imaginary axis and $2n - 2l$ eigenvalues off this axis.

Introducing bases in the corresponding invariant subspaces we can transform A to block diagonal form

$$A(L, R) = (L, R)\begin{pmatrix} A_h & 0 \\ 0 & A_c \end{pmatrix}, \quad L \in \mathbb{R}^{2n,2n-2l},\ R \in \mathbb{R}^{2n,2l}, \tag{1.2}$$

where $\Re\sigma(A_h) \neq 0$ and $\Re\sigma(A_c) = 0$ and the matrix $\Phi = (L, R)$ is symplectic in the sense

$$\Phi^T J^{-1}\Phi = \begin{pmatrix} L^T J^{-1}L & L^T J^{-1}R \\ R^T J^{-1}L & R^T J^{-1}R \end{pmatrix} = \begin{pmatrix} J^{-1}_{n-l} & 0 \\ 0 & J^{-1}_l \end{pmatrix}. \tag{1.3}$$

Here we use the canonical forms

$$J_\nu = \begin{pmatrix} 0 & I_\nu \\ -I_\nu & 0 \end{pmatrix} \quad \text{for } \nu = n - l, l.$$

The columns of L and R span symplectic subspaces of $\mathbb{R}^{2n}$ which are symplectic orthogonal to each other (see [7] for the linear theory).

It is well known from Mielke's book [8] that center manifolds of Hamiltonian systems keep a symplectic structure and that the reduced system can be put into Hamiltonian form again. In this paper we use the fact that the center manifold can be locally parametrized by a function

$$x = f(\omega), \quad \omega \in \mathbb{R}^{2l}, \tag{1.4}$$

where $f : \mathbb{R}^{2l} \to \mathbb{R}^{2n}$ is a symplectic mapping in the sense

$$\big(f'(\omega)\big)^T J^{-1} f'(\omega) = J_l^{-1}. \tag{1.5}$$

Such a representation follows by combining center manifold theory for the general case [3] with Darboux's theorem (cf. [1]); see Section 2 for more details. The reduced equation then assumes the canonical form

$$\dot\omega = J_l \nabla M(\omega), \quad \omega \in \mathbb{R}^{2l}, \text{ where } M = H \circ f.$$

The invariance condition for the manifold may be written as

$$f'(\omega) J_l \big(f'(\omega)\big)^T \nabla H\big(f(\omega)\big) = J\nabla H\big(f(\omega)\big). \tag{1.6}$$

It is well known that expansions of $f(\omega)$ of arbitrary order can be obtained from this condition in combination with the symplecticity requirement (1.5); see [8, Chapter 4.3].

It is the purpose of this paper to show how successive derivatives of $f(\omega)$ can be extracted from (1.5) and (1.6) subject to the following constraints:

- Only the (generally low-dimensional) matrices A_c, R are used in the algorithm (A_h, L are not needed);

- The linear algebra reduces to solving a series of bordered linear systems of the type

$$\begin{bmatrix} H_{uu}^0 - \lambda J^{-1} & J^{-1}R \\ -R^T J^{-1} & 0 \end{bmatrix} \begin{bmatrix} h \\ \varepsilon \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix},$$
$$\lambda \in \left\{ \sum_{j=1}^{k} \lambda_j \;\middle|\; \lambda_j \in \sigma(A_c),\ k \in \mathbb{N} \right\}. \tag{1.7}$$

Notice that the matrix in the bordered system (1.7) is Hermitian since $\lambda \in i\mathbb{R}$. Moreover, the principal submatrix $H_{uu}^0 - \lambda J^{-1}$ can be singular, but we will prove that the full matrix is nonsingular. For a stable and efficient solution of such systems one may use the mixed block elimination method of Govaerts (see [4,5]) combined with a sparse solver for the Hermitian principal submatrix. Our results can be considered as a special adaptation of the general method from [2] to the Hamiltonian case.

In Section 2 we prepare the computational procedure in such a way that only the matrices A, A_c appear and that the freedom in choosing the canonical transformation $x = f(\omega)$ becomes transparent. In Section 3 we eliminate this degree of freedom by a specific choice of parameters and we develop the algorithmic details for this case. Finally, as an example we apply the algorithm to a discretized version of an elliptic system in a strip.

2. The reduction procedure

In a first step we show that it is sufficient to solve the symplecticity condition (1.5) together with a $(2n - 2l)$-dimensional subsystem of Eq. (1.6).

For that purpose we introduce the decompositions

$$x = Lx_h + Rx_c = \Phi \begin{pmatrix} x_h \\ x_c \end{pmatrix}, \quad z = \begin{pmatrix} x_h \\ x_c \end{pmatrix}, \quad x_h \in \mathbb{R}^{2n-2l},\ x_c \in \mathbb{R}^{2l}, \tag{2.1}$$

and the new functions G, g via

$$G(z) = H(\Phi z), \qquad f = \Phi g = (L, R) \begin{pmatrix} g_h \\ g_c \end{pmatrix}. \tag{2.2}$$

The index c is used to indicate the central part which will be low-dimensional and the index h indicates the hyperbolic and normally high-dimensional part.

We require $f'(0) = R$, i.e.,

$$g_h'(0) = 0 \quad \text{and} \quad g_c'(0) = I_{2l}. \tag{2.3}$$

Using this decomposition and (1.3), Eq. (1.5) turns into

$$\big(g_h'(\omega)\big)^T \cdot J_{n-l}^{-1} g_h'(\omega) + \big(g_c'(\omega)\big)^T \cdot J_l^{-1} g_c'(\omega) = J_l^{-1} \tag{2.4}$$

and Eq. (1.6) may be written as

$$g'(\omega) \cdot J_l \big(g'(\omega)\big)^T \nabla G\big(g(\omega)\big) = \operatorname{diag}\{J_{n-l}, J_l\} \nabla G\big(g(\omega)\big) \tag{2.5}$$

or equivalently

$$g_h'(\omega) \cdot J_l\big(g'(\omega)\big)^T \nabla G\big(g(\omega)\big) = J_{n-l} \nabla_{x_h} G\big(g(\omega)\big), \tag{2.6}$$

$$g_c'(\omega) \cdot J_l\big(g'(\omega)\big)^T \nabla G\big(g(\omega)\big) = J_l \nabla_{x_c} G\big(g(\omega)\big). \tag{2.7}$$

In the following we show that it is sufficient to solve (2.4) and (2.6).

Lemma 2.1. *Assuming the symplectic condition* (2.4)*, the two Eqs.* (2.5) *and* (2.6) *are equivalent.*

Proof. It is sufficient to prove that (2.4) and (2.6) imply (2.7). In the first step we show that $\nabla_{x_h} G$ can be expressed in terms of $\nabla_{x_c} G$ as follows:

$$\nabla_{x_h} G \circ g = J_{n-l}^{-1} g_h' g_c'^{-1} J_l \nabla_{x_c} G \circ g, \tag{2.8}$$

where $g_h' = g_h'(\omega)$, $g_c' = g_c'(\omega)$. Notice that g_c' and $g_h' J_l g_h'^T - J_{n-l}$ are invertible near 0 due to (2.3). Rearranging terms in (2.6) we obtain

$$\big(g_h' J_l g_h'^T - J_{n-l}\big) \nabla_{x_h} G \circ g = -g_h' J_l g_c'^T \nabla_{x_c} G \circ g.$$

Equation (2.8) is then a consequence of the identity

$$\big(g_h' J_l g_h'^T - J_{n-l}\big)^{-1} g_h' J_l g_c'^T = J_{n-l} g_h' g_c'^{-1} J_l.$$

The last equation is equivalent to

$$g_h' J_l g_c'^T J_l^{-1} g_c' = \big(g_h' J_l g_h'^T - J_{n-l}\big) J_{n-l} g_h'$$

which follows by substituting $g_c'^T J_l^{-1} g_c'$ from (2.4).

Another consequence of (2.4) is

$$g_h'^T J_{n-l}^{-1} g_h' g_c'^{-1} J_l = \big(J_l^{-1} g_c'^{-1} - g_c'^T J_l^{-1}\big) J_l = J_l^{-1} g_c'^{-1} J_l - g_c'^T.$$

Apply this to $\nabla_{x_c} G$ and use (2.8) to obtain

$$g_h'^T \nabla_{x_h} G \circ g = \big(J_l^{-1} g_c'^{-1} J_l - g_c'^T\big) \nabla_{x_c} G \circ g.$$

Then multiply by $g_c' J_l$ from the left and rearrange to find our assertion (2.7) in the form

$$g_c' J_l\big(g_h^T G_{x_h} \circ g + g_c'^T G_{x_c} \circ g\big) = J_l \nabla_{x_c} G \circ g. \qquad \square$$

In the following our goal is to derive a recursion for the monomials in the formal Taylor expansion of the center manifold. This will be done in such a way that the large matrices L and A_h do not appear and only linear systems with a bordering of the original matrix A have to be solved.

Define $\mathcal{P}(Y, i)$ to be the space of homogeneous polynomials of degree i from $\mathbb{R}^{2l}$ into some vector space Y. It will be convenient to introduce the homogeneous polynomials

$$f_i(\omega) = \frac{1}{i!} f^{(i)}(0)\omega^i, \quad \phi_i(\omega) = \frac{1}{i!} L g_h^{(i)}(0)\omega^i, \quad \psi_i(\omega) = \frac{1}{i!} g_c^{(i)}(0)\omega^i, \tag{2.9}$$

for which $f_i \in \mathcal{P}(\mathbb{R}^{2n}, i)$, $\phi_i \in \mathcal{P}(\mathrm{Range}(L), i)$, $\psi_i \in \mathcal{P}(\mathbb{R}^{2l}, i)$ and the relation $f_i = \phi_i + R\psi_i$ holds according to (2.2).

For the computation of these coefficients, we have the following necessary condition. A certain converse will be discussed in the subsequent theorem.

Theorem 2.2. *Let $x = f(\omega)$ define any smooth center manifold of* (1.1) *that satisfies* (2.2)–(2.4) *and consider the decomposition of its Taylor terms*

$$f_i = \phi_i + R\psi_i, \quad \text{where } \phi_i \in \mathcal{P}\big(\mathrm{Range}(L), i\big),\ \psi_i \in \mathcal{P}(\mathbb{R}^{2l}, i). \tag{2.10}$$

Then there exist unique polynomials $q_i = q_i(\omega) \in \mathcal{P}(\mathbb{R}, i+1)$ such that the following set of recursive equations holds for $i \geqslant 2$:

$$\psi_i = \frac{1}{2} J_l \sum_{r=1}^{i-2} \big(\psi_{r+1}'^{T} J_l \psi_{i-r} - \phi_{r+1}'^{T} J^{-1} \phi_{i-r}\big) - J_l \nabla q_i, \tag{2.11}$$

$$\phi_i'(\omega) A_c \omega - A\phi_i(\omega) = T_i, \quad R^T J^{-1} \phi_i(\omega) = 0. \tag{2.12}$$

Here the functions $T_i \in \mathcal{P}(\mathrm{Range}(L), i)$ are uniquely determined by ϕ_j, ψ_j, $j = 1, \dots, i-1$ (*see* (2.21) *below for an explicit formula*).

Remark. The freedom in choosing the polynomials q_i originates from the fact that the parametrization $x = f(\omega)$ in (1.4) is only unique up to a symplectic change of coordinates ω.

Proof of Theorem 2.2. For convenience we introduce the abbreviations

$$S_{i,h}(\omega) = \frac{1}{i!} g_h^{(i)}(0)\omega^i, \quad S_i(\omega) = \frac{1}{i!} g^{(i)}(0)\omega^i, \quad G(z) = \sum_{i=2}^{+\infty} \frac{1}{i!} G^{(i)}(0) z^i. \tag{2.13}$$

Using (2.13) Eq. (2.6) may be rewritten as follows:

$$\left\{\left(\sum_{i=1}^{+\infty} S_{i,h}'(\omega)\right) J_l \left(\sum_{i=1}^{+\infty} S_i'(\omega)\right)^T - [J_{n-l}, 0]\right\} \sum_{i=1}^{+\infty} \frac{1}{i!} G^{(i+1)}(0) \left(\sum_{l=1}^{+\infty} S_l(\omega)\right)^i = 0, \tag{2.14}$$

where 0 in $[J_{n-l}, 0]$ is a zero matrix with $2(n-l)$ rows and $2l$ columns. With a slight abuse of notation we use here and in the following the notation $y = G^{(i+1)}(0)(z_1, \dots, z_i)$ for the vector defining the linear form $y^T x = G^{(i+1)}(0)(z_1, \dots, z_i, x)$. Notice that $S_{1,h}'(\omega) = 0$ and $\psi_1'(\omega) = I_{2l}$, so (2.4) and (2.9) lead to

$$\sum_{i=2}^{+\infty} \big[J_l \psi_i' - (J_l \psi_i')^T\big] + \sum_{i=2}^{+\infty} \psi_i'^{T} J_l \sum_{i=2}^{+\infty} \psi_i' + \sum_{i=2}^{+\infty} S_{i,h}'^{T} J_{n-l} \sum_{i=2}^{+\infty} S_{i,h}' = 0. \tag{2.15}$$

Comparing coefficients in (2.15) we obtain $J_l \psi_2' - (J_l \psi_2')^T = 0$ and when $i \geqslant 3$,

$$J_l \psi_i' - (J_l \psi_i')^T + \sum_{r=1}^{i-2} \big(\psi_{r+1}'^{T} J_l \psi_{i-r}' + S_{r+1,h}'^{T} J_{n-l} S_{i-r,h}'\big) = 0,$$

$$J_l \psi_i' - (J_l \psi_i')^T + \sum_{r=1}^{i-2} \big(\psi_{r+1}'^{T} J_l \psi_{i-r}' - (L S_{r+1,h}')^T J^{-1} L S_{i-r,h}'\big) = 0. \tag{2.16}$$

By (2.9) and (2.13) we know that $LS'_{i,h} = \phi'_i$, so (2.16) becomes

$$J_l\psi'_i - (J_l\psi'_i)^T + \sum_{r=1}^{i-2}\left(\psi'^T_{r+1}J_l\psi'_{i-r} - \phi'^T_{r+1}J^{-1}\phi'_{i-r}\right) = 0.$$

Let $\mathrm{Sym}(2l)$ denote the set of $2l \times 2l$ symmetric matrices, then

$$J_l\psi'_2 \in \mathrm{Sym}(2l)$$

and

$$J_l\psi'_i + \frac{1}{2}\sum_{r=1}^{i-2}\left(\psi'^T_{r+1}J_l\psi'_{i-r} - \phi'^T_{r+1}J^{-1}\phi'_{i-r}\right) \in \mathrm{Sym}(2l) \quad (i > 2).$$

Take

$$K_2 = J_l\psi_2, \quad K_i = J_l\psi_i + \frac{1}{2}\sum_{r=1}^{i-2}\left(\psi'^T_{r+1}J_l\psi_{i-r} - \phi'^T_{r+1}J^{-1}\phi_{i-r}\right) \quad (i > 2),$$

then $K'_2 = J_l\psi'_2 \in \mathrm{Sym}(2l)$ and

$$K'_i = J_l\psi'_i + \frac{1}{2}\sum_{r=1}^{i-2}\left(\psi'^T_{r+1}J_l\psi'_{i-r} - \phi'^T_{r+1}J^{-1}\phi'_{i-r}\right) \in \mathrm{Sym}(2l) \quad (i > 2).$$

Hence we find $K_i = \nabla q_i$ for some unique $q_i \in \mathcal{P}(\mathbb{R}, i+1)$, i.e.,

$$\psi_2 = -J_l\nabla q_2,$$
$$\psi_i = \frac{1}{2}J_l\sum_{r=1}^{i-2}\left(\psi'^T_{r+1}J_l\psi_{i-r} - \phi'^T_{r+1}J^{-1}\phi_{i-r}\right) - J_l\nabla q_i \quad (i > 2).$$

Next we solve for $S_{i,h}$, and compare coefficients in (2.14). The term of degree i involves $S_{i,h}$ in the form

$$\begin{aligned} &S'_{i,h}(\omega)J_lS'^T_1G^{(2)}(0)S_1(\omega) - [J_{n-l}, 0]G^{(2)}(0)S_i(\omega) \\ &\quad = S'_{i,h}A_c\omega - A_hS_{i,h}(\omega). \end{aligned} \tag{2.17}$$

To see this, observe that by (1.2) and (1.3) and $A = JH^{(2)}(0)$, we have

$$\begin{aligned} \Phi^TH^{(2)}(0)\Phi &= \Phi^TJ^{-1}\Phi\cdot\Phi^{-1}JH^{(2)}(0)\Phi = \Phi^TJ^{-1}\Phi\cdot\Phi^{-1}A\Phi \\ &= \mathrm{diag}\left\{J^{-1}_{n-l}, J^{-1}_l\right\}\mathrm{diag}\{A_h, A_c\} = \mathrm{diag}\left\{J^{-1}_{n-l}A_h, J^{-1}_lA_c\right\}. \end{aligned}$$

From $G = H \circ \Phi$, we further obtain

$$G^{(2)}(0) = \Phi^TH^{(2)}(0)\Phi = \mathrm{diag}\left\{J^{-1}_{n-l}A_h, J^{-1}_lA_c\right\}. \tag{2.18}$$

Using $S_1(\omega) = g'(0)\omega$, $g'^T(0) = [0, I_{2l}]$ and (2.18), we get

$$\begin{aligned}
&S'_{i,h}(\omega)J_l S_1'^T G^{(2)}(0)S_1(\omega) - [J_{n-l},0]G^{(2)}(0)S_i(\omega)\\
&\quad = S'_{i,h}(\omega)J_l[0,I_{2l}]\operatorname{diag}\left\{J_{n-l}^{-1}A_h, J_l^{-1}A_c\right\}[0,I_{2l}]^T\omega\\
&\qquad - [J_{n-l},0]\operatorname{diag}\left\{J_{n-l}^{-1}A_h, J_l^{-1}A_c\right\}S_i(\omega)\\
&\quad = S'_{i,h}(\omega)A_c\omega - \operatorname{diag}\{A_h,0\}S_i(\omega)\\
&\quad = S'_{i,h}(\omega)A_c\omega - A_h S_{i,h}(\omega),
\end{aligned}$$

hence (2.17) holds.

Collecting the other terms leads to

$$S'_{i,h}A_c\omega - A_h S_{i,h} = \tilde{T}_{i,h}, \tag{2.19}$$

where

$$\begin{aligned}
\tilde{T}_{i,h} = [J_{n-l},0]&\Biggl[\sum_{j=2}^{i}\frac{1}{j!}\sum_{r_1+r_2+\cdots+r_j=i} G^{(j+1)}(0)(S_{r_1},S_{r_2},\ldots,S_{r_j})\Biggr]\\
&- \sum_{r=1}^{i-2} S'_{r+1,h}J_l S_{i-r}'^T G^{(2)}(0)S_1 - \sum_{k=3}^{i}\left(\sum_{r=1}^{k-1} S'_{r,h}J_l S_{k-r}'^T\right)\\
&\times\Biggl[\sum_{j=1}^{i+2-k}\frac{1}{j!}\sum_{r_1+r_2+\cdots+r_j=i+2-k} G^{(j+1)}(0)(S_{r_1},S_{r_2},\ldots,S_{r_j})\Biggr].
\end{aligned}$$

Multiplying by L we may write (2.19) equivalently as

$$\phi_i' A_c\omega - A\phi_i = T_i, \quad R^T J^{-1}\phi_i = 0, \tag{2.20}$$

where $T_i = L\tilde{T}_{i,h}$ can now be expressed in terms of the original Hamiltonian function as follows:

$$\begin{aligned}
T_i = (J - RJ_lR^T)&\Biggl[\sum_{j=2}^{i}\frac{1}{j!}\sum_{r_1+r_2+\cdots+r_j=i} H^{(j+1)}(0)(f_{r_1},f_{r_2},\ldots,f_{r_j})\Biggr]\\
&- \sum_{r=1}^{i-2}\phi'_{r+1}J_l f_{i-r}'^T H^{(2)}(0)f_1 - \sum_{k=3}^{i}\left(\sum_{r=1}^{k-1}\phi'_r J_l f_{k-r}'^T\right)\\
&\times\Biggl[\sum_{j=1}^{i+2-k}\frac{1}{j!}\sum_{r_1+r_2+\cdots+r_j=i+2-k} H^{(j+1)}(0)(f_{r_1},f_{r_2},\ldots,f_{r_j})\Biggr].
\end{aligned} \tag{2.21}$$

Notice that we used the equality $LJ_{n-l}L^T = J - RJ_lR^T$ in order to write everything in terms of low-dimensional matrices. □

We will now show that the necessary conditions from Theorem 2.2 with arbitrarily chosen q_i can be used to approximate center manifolds to any given order.

We recall that, by definition, a center manifold of (1.1) is a locally invariant manifold that contains the origin and is tangent to the subspace $\mathrm{Range}(R)$. It is well known that center manifolds are generally nonunique but their Taylor expansions are unique (cf. [3]).

Moreover, in the Hamiltonian case, any center manifold can be parametrized by a symplectic mapping (cf. (1.4) and (1.5)).

The following algorithm collects the main information from Theorem 2.2. It is preliminary in the sense that an implementation for large systems needs more details. These will be developed in the next section.

Algorithm. Compute $\psi_i \in \mathcal{P}(\mathbb{R}^{2l}, i)$, $\phi_i \in \mathcal{P}(\mathrm{Range}(L), i)$ inductively for $i \geqslant 1$ as follows:

(1) Define $\psi_1 = \omega$, $\phi_1 = 0$,
(2) (a) determine $T_i \in \mathcal{P}(\mathrm{Range}(L), i)$, $i \geqslant 2$, from (2.21),
 (b) choose $q_i \in \mathcal{P}(\mathbb{R}, i+1)$ arbitrarily,
 (c) compute $\phi_i \in \mathcal{P}(\mathrm{Range}(L), i)$ as the unique solution of (2.12),
 (d) define ψ_i by (2.11).

For this algorithm, we have the following result.

Theorem 2.3. *Let the system* (1.1) *satisfy assumptions* (1.2) *and* (1.3)*. Then the following holds*:

(a) *Any center manifold of type C^m, $m \geqslant 2$, can be locally parametrized by a symplectic mapping $x = f(\omega)$ as in* (1.4) *and* (1.5).
(b) *For any sequence $q_i \in \mathcal{P}(\mathbb{R}, i+1)$ and ϕ_i, ψ_i determined by the algorithm above and for any index m, there exists a center manifold $x = f(\omega)$ such that* (1.5) *holds and*

$$f(\omega) = \sum_{i=1}^{m} f_i(\omega) + o\big(|\omega|^m\big), \quad \text{where } f_i = \phi_i + R\psi_i. \tag{2.22}$$

Proof. (a) By the linear transformation (2.1)–(2.2) we may write (1.1) as

$$\dot{x}_h = J_{n-l}\nabla_{x_h} G(x_h, x_c), \qquad \dot{x}_c = J_l \nabla_{x_c} G(x_h, x_c).$$

From classical theory (see [3]), for any $m > 0$, there exists a center manifold of graph type $(h(v), v)$, where $h \in C^m(\mathbb{R}^{2l}, \mathbb{R}^{2n-2l})$, $h(0) = 0$, $h'(0) = 0$ and

$$J_{n-l} G_{x_h}^T\big(h(v), v\big) = h' J_l \nabla_{x_c} G\big(h(v), v\big). \tag{2.23}$$

Now Darboux's theorem (see [1]) yields a local diffeomorphism $\rho \in C^{m-1}(\mathbb{R}^{2l}, \mathbb{R}^{2l})$ such that

$$J_l + h'^T(x_c) J_{n-l} h' = \rho'(x_c)^T J_l \rho'(x_c).$$

Setting $g_c(\omega) = \rho^{-1}(\omega)$, $g_h(\omega) = h \circ \rho^{-1}(\omega)$ one then easily verifies $g_h'^T J_{n-l} g_h' + g_c' J_l g_c' = J_l$. From this one obtains that $f(\omega) = L g_h(\omega) + R g_c(\omega)$ parametrizes the given center manifold and satisfies (1.5).

(b) Next we prove that (2.19) and hence the equivalent Eq. (2.20) has a unique solution. Let $E_i = \mathcal{P}(\mathbb{R}^{2n-2l}, i)$ and $\Phi_i : E_i \to E_i$ be the following linear mapping:

$$\big(\Phi_i(x)\big)(\omega) = x'(\omega) A_c \omega - A_h x(\omega).$$

It is enough to show that $\Phi_i(x) = 0$ has only the zero solution. Taking the ith derivative of $\Phi_i(x)$ we obtain that $X := x^{(i)}$ satisfies

$$\sum_{j=1}^{i} X(h_1, \dots, A_c h_j, \dots, h_i) - A_h X(h_1, \dots, h_i) = 0$$

for all $h_j \in \mathbb{R}^{2n-2l}$, $j = 1, \dots, i$. Since $\sigma(A_h) \cap \{\sum_{j=1}^{i} \lambda_j \mid \lambda_j \in \sigma(A_c)\} = \emptyset$, we conclude $X = 0$ by a result on multilinear Sylvester equations in [2]. Thus $x = 0$ and the solvability is proved.

Proving the existence of a center manifold $x = f(\omega)$, satisfying (2.22) follows by combining the existence proof above with the calculations in Theorem 2.2. Therefore we merely indicate the main steps.

(1) With ψ_i, ϕ_i calculated from (2.11) and (2.12) define

$$\tilde{g}_c = \sum_{i=1}^{m} \psi_i, \quad \tilde{g}_h = J_{n-l} L^T J^{-1} \sum_{i=1}^{m} \phi_i, \quad \tilde{h} = \tilde{g}_h \circ \tilde{g}_c^{-1}$$

and notice $L\tilde{g}_h = \sum_{i=1}^{m} \phi_i$. Reversing the arguments in Theorem 2.2 leads to

$$J_{n-l} G_{x_h}^T\big(\tilde{h}(v), v\big) = \tilde{h}' J_l \nabla_{x_c} G\big(\tilde{h}(v), v\big) + o(v^m).$$

Comparing this with a given center manifold $(h(v), v)$ that satisfies (2.23) we conclude from [3] the relation

$$h(v) - \tilde{h}(v) = o(\omega^m) \quad \text{and} \quad h'(v) - \tilde{h}'(v) = o(\omega^{m-1}).$$

(2) Let $\bar{g}_c = \tilde{g}_c$, $\bar{g}_h = h \circ \tilde{g}_c$; then by a straightforward calculation

$$\big(\bar{g}_h'(\omega)\big)^T \cdot J_{n-l}^{-1} \bar{g}_h'(\omega) + \big(\bar{g}_c'(\omega)\big)^T \cdot J_l^{-1} \bar{g}_c'(\omega) = J_l^{-1} + B_1(\omega),$$

where $B_1(\omega) = o(\omega^{m-1})$. Thus we know that the 2-form corresponding to $J_l^{-1} + B_1(\omega)$ is closed and nondegenerate when ω is small.

(3) Using the method of proof from Darboux's theorem in [1], we can prove that there is a function $\tilde{\rho} \in C^{m-1}(\mathbb{R}^{2l}, \mathbb{R}^{2l})$ such that $\tilde{\rho}(\omega) = \omega + o(\omega^m)$ and

$$\tilde{\rho}'^T(\omega) J_l^{-1} \tilde{\rho}'(\omega) = J_l^{-1} + B_1(\omega).$$

(4) With the settings $g_c = \tilde{g}_c \circ \tilde{\rho}^{-1}$, $g_h = h \circ g_c$, we then find that $f = Lg_h + Rg_c$ has the desired properties. □

Remark. The basic equation (2.12) which appears in our algorithm is also fundamental in the calculation of normal forms for a given Hamiltonian (compare [10] and [8, Chapter 4.3]). Notice, however, that in our formulation (2.12) the original linearization A appears unchanged. Moreover, Taylor expansions of the reduced Hamiltonian $M(\omega) = H(f(\omega))$ can easily be computed from the Taylor expansion of f. This will not be carried out in general, but we will show such a computation for the example in Section 4.

3. The algorithm

In this section we discuss the details of the implementation of the algorithm developed in the previous section. First we note that we can remove the arbitrariness in the parametrization by setting $q_i = 0$. Then the Taylor coefficients $\psi_i, \phi_i, f_i, i \geqslant 2$, can be determined from

$$\psi_i = \frac{1}{2} J_l \sum_{r=1}^{i-2} \left(\psi_{r+1}'^T J_l \psi_{i-r} - \phi_{r+1}'^T J^{-1} \phi_{i-r}\right), \tag{3.1}$$

$$\phi_i'(\omega) A_c \omega - A\phi_i(\omega) = T_i, \quad R^T J^{-1} \phi_i(\omega) = 0, \tag{3.2}$$

$$f_i = \phi_i + R\psi_i. \tag{3.3}$$

Here the expressions T_i are defined in terms of ψ_j, ϕ_j $(j \leqslant i-1)$ through (2.21). In the following we show how the recursion (3.1)–(3.3) can be turned into a practical algorithm by using the Schur normal form of A_c and by solving a sequence of bordered linear systems.

Consider the Schur normal form of A_c,

$$P^{-1} A_c P = B = \begin{bmatrix} b_{1,1} & b_{1,2} & \cdots & b_{1,2l} \\ & b_{2,2} & \cdots & b_{2,2l} \\ & & \ddots & \vdots \\ & & & b_{2l,2l} \end{bmatrix}, \quad P \text{ is unitary},$$

where $b_{p,p} \in i\mathbb{R}$, $p = 1, \dots, 2l$, are the eigenvalues of A_c. Let $\omega = Py$ and define for later reference

$$\bar{\phi}_i(y) = \phi_i(Py) = \sum_{|\nu|=i} \bar{\phi}_\nu y^\nu \quad \text{and} \quad \bar{T}_i(y) = T_i(Py) = \sum_{|\nu|=i} \bar{T}_\nu y^\nu. \tag{3.4}$$

For convenience we use here the same symbol to denote the function and its Taylor coefficients and we suppress the dependence of the coefficients on i. With this notation, Eq. (3.2) now reads

$$\bar{\phi}_i'(y) By - A\bar{\phi}_i(y) = \bar{T}_i(y), \quad R^T J^{-1} \bar{\phi}_i(y) = 0$$

and may be rewritten explicitly as

$$\sum_{|\nu|=i} \bar{\phi}_\nu y^\nu \left(\frac{\nu_1}{y_1}, \dots, \frac{\nu_{2l}}{y_{2l}}\right) By - \sum_{|\nu|=i} A\bar{\phi}_\nu y^\nu = \bar{T}_i(y), \quad R^T J^{-1} \bar{\phi}_\nu = 0, \tag{3.5}$$

where

$$\left(\frac{\nu_1}{y_1}, \dots, \frac{\nu_{2l}}{y_{2l}}\right) By = \lambda_\nu + \sum_{1 \leqslant k < j \leqslant 2l} b_{k,j} \nu_k \frac{y_j}{y_k}, \quad \lambda_\nu = \sum_{j=1}^{2l} b_{j,j} \nu_j.$$

For $k < j$ let

$$\alpha_{k,j}(\nu) = (\nu_1, \dots, \nu_{k-1}, \nu_k - 1, \nu_{k+1}, \dots, \nu_{j-1}, \nu_j + 1, \nu_{j+1}, \dots, \nu_{2l}). \tag{3.6}$$

Then (3.5) becomes

$$\sum_{|\nu|=i} d(\nu) y^\nu - \sum_{|\nu|=i} A\bar{\phi}_\nu y^\nu = \bar{T}_i(y), \quad R^T J^{-1}\bar{\phi}_\nu = 0, \tag{3.7}$$

where $d(\nu) = \lambda_\nu \bar{\phi}_\nu + \sum_{1 \leqslant k<j \leqslant 2l} b_{k,j}(1+\nu_k)\bar{\phi}_{\alpha_{k,j}^{-1}(\nu)}$.

Notice that in this sum only summands with $\nu_j \geqslant 1$ occur since

$$\alpha_{k,j}^{-1}(\nu) = (\nu_1, \ldots, \nu_{k-1}, \nu_k + 1, \nu_{k+1}, \ldots, \nu_{j-1}, \nu_j - 1, \nu_{j+1}, \ldots, \nu_{2l}).$$

Comparing coefficients in (3.7) leads to the equation

$$\lambda_\nu \bar{\phi}_\nu - A\bar{\phi}_\nu = \bar{T}_\nu - \sum_{1 \leqslant k<j \leqslant 2l} b_{k,j}(1+\nu_k)\bar{\phi}_{\alpha_{k,j}^{-1}(\nu)}, \quad R^T J^{-1}\bar{\phi}_\nu = 0. \tag{3.8}$$

These systems can be solved in a reverse lexicographical order so that $\bar{\phi}_{\alpha_{k,j}^{-1}(\nu)}$ is known when $\bar{\phi}_\nu$ is to be computed. In order to solve (3.8) in a stable way, we introduce extra unknowns $\varepsilon_\nu \in \mathbb{R}^{2l}$ and use the equations

$$(A - \lambda_\nu)\bar{\phi}_\nu + R\varepsilon_\nu = \sum_{1 \leqslant k<j \leqslant 2l} b_{k,j}(1+\nu_k)\bar{\phi}_{\alpha_{k,j}^{-1}(\nu)} - \bar{T}_\nu, \quad R^T J^{-1}\bar{\phi}_\nu = 0. \tag{3.9}$$

Because $\bar{T}_\nu \in \mathrm{Range}(L)$ we will have $\varepsilon_\nu = 0$, $\bar{\phi}_\nu \in \mathrm{Range}(L)$ for the solution of (3.9). The bordering by R is only included to account for numerical errors in the terms $\bar{T}_\nu$. The matrix form of (3.9) is

$$C_\nu X_\nu = Y_\nu, \tag{3.10}$$

where

$$C_\nu = \begin{bmatrix} A - \lambda_\nu & R \\ -R^T J^{-1} & 0 \end{bmatrix}, \qquad X_\nu = \begin{bmatrix} \bar{\phi}_\nu \\ \varepsilon_\nu \end{bmatrix},$$

$$Y_\nu = \begin{bmatrix} \sum_{1 \leqslant k<j \leqslant 2l} b_{k,j}(1+\nu_k)\bar{\phi}_{\alpha_{k,j}^{-1}(\nu)} - \bar{T}_\nu \\ 0 \end{bmatrix}.$$

Finally, we rewrite (3.10) by multiplying with $Z = \mathrm{diag}\{J^{-1}, I_{2l}\}$ to obtain

$$D_\nu X_\nu = Z Y_\nu,$$

where

$$D_\nu = \begin{bmatrix} H_{uu}^0 + \lambda_\nu J^{-1} & J^{-1}R \\ -R^T J^{-1} & 0 \end{bmatrix}$$

is a Hermitian matrix due to $\Re\sigma(A_c) = 0$.

Lemma 3.1. *The matrix C_ν is nonsingular if $\lambda_\nu \notin \sigma(A_h)$.*

Proof. We show that the equation $C_\nu X_\nu = 0$ has only the zero solution. Suppose that

$$(A - \lambda_\nu)\bar{\phi}_\nu + R\varepsilon_\nu = 0, \tag{3.11}$$

$$R^T J^{-1}\bar{\phi}_\nu = 0. \tag{3.12}$$

By (3.12) we know that $\bar{\phi}_\nu = Ly$ for some $y \in \mathbb{R}^{2n-2l}$, insert it into (3.11) and multiply by $L^T J^{-1}$ from the left to obtain

$$L^T J^{-1}(A - \lambda_\nu)Ly + L^T J^{-1} R\varepsilon_\nu = 0.$$

Since $L^T J^{-1} R = 0$, $AL = LA_h$ and $L^T J^{-1} L = J_{n-l}^{-1}$, we have that

$$J_{n-l}^{-1}(A_h - \lambda_\nu)y = 0.$$

From our hypothesis we find that $y = 0$ hence $\bar{\phi}_\nu = 0$, and (3.11) yields $\varepsilon_\nu = 0$ because R has full rank. □

4. Application to an elliptic system

By the results of last section, we have reduced the problem of approximating a center manifold to solving Eq. (3.10) with $\bar{T}_i$ defined by (3.4) and (2.21). The number of such linear equations is $\binom{2l+i-1}{2l-1}$, where i is the degree of ω.

In this section we will carry through the algorithm for a semi-discretization of the following elliptic system in a strip $x \in [0, 1]$, $t \in \mathbb{R}$:

$$\begin{aligned} &u_{tt} + u_{xx} + F(u) = 0, \\ &u(t, 0) = u(t, 1) = 0. \end{aligned} \tag{4.1}$$

We assume $F \in C^1(\mathbb{R}, \mathbb{R})$, $F(0) = 0$ and $F'(0) > \pi^2$. We apply the so-called *spatial center manifold theory* which originates from a paper of Kirchgässner [6] (see [8,9] for the further development). That is, we write the system as a dynamical system in the unbounded variable t (this leads to unbounded spectra on both sides of the imaginary axis) and use a center manifold reduction with respect to this variable.

Center manifold reduction is one of the well-known methods for studying all bounded and small solutions of elliptic systems such as (4.1) in spite of the fact that, considered as an evolutionary equation, this system is not well posed.

First we discretize (4.1) in x-direction by introducing

$$x_j = jh, \quad j = 0, 1, \ldots, n, \ h = \frac{1}{n}, \qquad u_j = u(t, x_j).$$

Then (4.1) is replaced by

$$\ddot{u}_j + \Delta_h u_j + F(u_j) = 0, \quad j = 1, \ldots, n-1, \ u_0 = u_n = 0,$$

where

$$\Delta_h u_j = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}, \quad j = 1, \ldots, n-1.$$

In matrix form we write this as

$$\ddot{U} + \frac{S - 2I}{h^2} U + F(U) = 0, \tag{4.2}$$

where

$$U=\begin{bmatrix} u_1\\ u_2\\ \vdots\\ u_{n-1}\end{bmatrix},\qquad S=\begin{bmatrix}0&1&&\\1&0&\ddots&\\&\ddots&\ddots&1\\&&1&0\end{bmatrix},\qquad F(U)=\begin{bmatrix}F(u_1)\\F(u_2)\\ \vdots\\ F(u_{n-1})\end{bmatrix}.$$

Let $V=\dot U$, then (4.2) becomes

$$\dot U=V,\qquad \dot V=\frac{2I-S}{h^2}U-F(U). \tag{4.3}$$

This system is of Hamiltonian form with

$$H(U,V)=\frac{1}{n}\left(\frac{1}{2}V^TV+F_1(U)+U^T\frac{S-2I}{2h^2}U\right),\quad F_1(U)=\sum_{k=1}^{n-1}\int_0^{u_k}F(v)\,dv,$$

and

$$J=\begin{bmatrix}0&nI_{n-1}\\-nI_{n-1}&0\end{bmatrix}.$$

Consider the Jacobian of (4.3) at the equilibrium point $U=0$,

$$A=\begin{bmatrix}0&I\\D&0\end{bmatrix},\quad D=\frac{2I-S}{h^2}-F'(0).$$

Since $\det(\lambda-A)=\det(\lambda^2-D)$ and D has only real eigenvalues the eigenvalues of A occur in pairs with opposite sign, either both real or both purely imaginary. The matrix S is known to be diagonalizable as follows:

$$S\eta=\eta\cdot\operatorname{diag}\{s_1,\dots,s_{n-1}\},\quad s_k=2\cos\frac{k\pi}{n},$$

where the orthogonal columns of the matrix η are given by

$$\eta_k=\sqrt{2}\left(\sin\frac{k\pi}{n},\sin\frac{2k\pi}{n},\dots,\sin\frac{(n-1)k\pi}{n}\right)^T.$$

Therefore, D is diagonalized by the same matrix and has eigenvalues

$$d_k=\frac{2-s_k}{h^2}-F'(0)=\left(2n\sin\frac{k\pi}{2n}\right)^2-F'(0).$$

We now choose numbers

$$l=l(n)=\left\lfloor\frac{2n}{\pi}\arcsin\left(\frac{\sqrt{F'(0)}}{2n}\right)\right\rfloor,\quad n\geqslant\left\lfloor\frac{\sqrt{F'(0)}}{2}\right\rfloor+1,$$

so that $d_1<\dots<d_l\leqslant 0<d_{l+1}<\dots<d_{n-1}$, where $\lfloor x\rfloor$ stands for the maximal number less equal x. When n increases, $l=l(n)$ decreases and tends to $\lfloor\sqrt{F'(0)}/\pi\rfloor$. Introducing the matrices $W_c=[\eta_1,\dots,\eta_l]$, $W_h=[\eta_{l+1},\dots,\eta_{n-1}]$, $D_c=\operatorname{diag}\{d_1,\dots,d_l\}$, $D_h=\operatorname{diag}\{d_{l+1},\dots,d_{n-1}\}$ we obtain the blockdiagonalization (1.2) with

$$\Phi=\begin{pmatrix}W_h&0&W_c&0\\0&W_h&0&W_c\end{pmatrix},\qquad A_h=\begin{pmatrix}0&I_{n-l}\\D_h&0\end{pmatrix},\qquad A_c=\begin{pmatrix}0&I_l\\D_c&0\end{pmatrix}.$$

The further details are displayed for the special nonlinearity

$$F(u) = 2\pi^2 u + 3u^2.$$

We assume $n \geqslant 3$ so that $l(n) = 1$ and

$$R = \begin{pmatrix} \eta_1 & 0 \\ 0 & \eta_1 \end{pmatrix}, \qquad A_c = \begin{pmatrix} 0 & 1 \\ d_1 & 0 \end{pmatrix}.$$

It is convenient to write

$$d_1 = -c^2, \quad \text{where } c = \left(F'(0) - \left(2n \sin \frac{\pi}{2n} \right)^2 \right)^{1/2}.$$

With the unitary and symplectic matrix

$$P = \frac{1}{\sqrt{1+c^2}} \begin{bmatrix} 1 & ic \\ ic & 1 \end{bmatrix}$$

we obtain

$$A_c P = PB, \quad \text{where } B = \begin{bmatrix} ic & 1-c^2 \\ 0 & -ic \end{bmatrix}.$$

With the coefficients $\bar{\phi}_\nu, \bar{T}_\nu$ from (3.4) and with the simplified index function $\alpha(\nu) = (\nu_1 - 1, \nu_2 + 1)$ (cf. (3.6)), Eq. (3.8) has the form

$$(\nu_1 + 1)(1 - c^2)\bar{\phi}_{\alpha^{-1}(\nu)} + (\lambda_\nu - A)\bar{\phi}_\nu = \bar{T}_\nu, \quad R^T J^{-1} \bar{\phi}_\nu = 0.$$

In the following recursive procedure we replace the index i by ι (to avoid a conflict with the complex unit i). During the computation of (ϕ_ι, ψ_ι) the coefficients of the following expansions appear:

$$T_\iota(\omega) = \sum_{|\nu|=\iota} T_\nu \omega^\nu, \qquad \bar{T}_\iota(y) = T_\iota(Py) = \sum_{|\nu|=\iota} \bar{T}_\nu y^\nu,$$

$$\phi_\iota(\omega) = \sum_{|\nu|=\iota} \phi_\nu \omega^\nu, \qquad \bar{\phi}_\iota(y) = \sum_{|\nu|=\iota} \bar{\phi}_\nu y^\nu, \qquad \phi'_\iota(\omega) = \sum_{|\nu|=\iota-1} \phi'_\nu \omega^\nu,$$

$$\psi_\iota(\omega) = \sum_{|\nu|=\iota} \psi_\nu \omega^\nu, \qquad \psi'_\iota(\omega) = \sum_{|\nu|=\iota-1} \psi'_\nu \omega^\nu,$$

$$f_\iota(\omega) = \sum_{|\nu|=\iota} f_\nu \omega^\nu = \phi_\iota(\omega) + R\psi_\iota(\omega),$$

$$f'_\iota(\omega) = \sum_{|\nu|=\iota-1} f'_\nu \omega^\nu = \phi'_\iota(\omega) + R\psi'_\iota(\omega).$$

We start with

$$\phi_1(\omega) = 0, \qquad \psi_1(\omega) = \omega, \qquad \psi_2(\omega) = 0$$

and perform for $\iota \geqslant 2$ the following three steps.

Step 1. *Computation of* $\bar{T}_\nu$, $|\nu| = \iota$.

Noticing that $H^{(k)} = 0$ for $k \geqslant 4$ and comparing coefficients of T_ι in (2.21) leads to the following expression:

$$\begin{aligned}
T_\nu = &- \sum_{(k,r,a_1,b_1)\in\bar{A}_\nu} \phi'_{(a_1,r-1-a_1)} J_l f'^{T}_{(b_1,k-r-1-b_1)} H^{(2)}(0) \\
&\times f_{(\nu_1-a_1-b_1,\iota+2-k-\nu_1+a_1+b_1)} \\
&- \frac{1}{2} \sum_{(k,r,s,a_1,b_1,d_1)\in\bar{B}_\nu} \phi'_{(a_1,r-1-a_1)} J_l f'^{T}_{(b-1,k-r-1-b_1)} H^{(3)}(0) f_{(d_1,s-d_1)} \\
&\times f_{(\nu_1-a_1-b_1-d_1,\iota+2-k-s-\nu_1+a_1+b_1+d_1)} \\
&- \sum_{(r,s_1,g_1)\in\bar{C}_\nu} \phi'_{(s_1,\nu_1-s_1)} J_l f'^{T}_{(g_1,\iota-r-1-g_1)} H^{(2)}(0) f_{(\nu_1-s_1-g_1,1-\nu_1+s_1+g_1)} \\
&+ \frac{1}{2} \sum_{(r,m_1)\in\bar{D}_\nu} (J - RJ_l R^T) H^{(3)}(0) f_{(m_1,r-m_1)} f_{(\nu_1-m_1,\iota-r-\nu_1+m_1)},
\end{aligned}$$

where we have used the following index sets:

$$\begin{aligned}
\bar{A}_\nu = \big\{&(k,r,a_1,b_1) \mid 3 \leqslant k \leqslant \iota,\ 1 \leqslant r \leqslant k-1,\ 0 \leqslant a_1 \leqslant \min(r-1,\nu_1), \\
&\max(0,\nu_1-(\iota+2-k)-a_1) \leqslant b_1 \\
&\leqslant \min(k-r-1,\nu_1-a_1)\big\}, \\
\bar{B}_\nu = \big\{&(k,r,s,a_1,b_1,d_1) \mid 3 \leqslant k \leqslant \iota,\ 1 \leqslant r \leqslant k-1,\ 0 \leqslant s \leqslant \iota+2-k, \\
&0 \leqslant a_1 \leqslant \min(r-1,\nu_1), \\
&0 \leqslant b_1 \leqslant \min(k-r-1,\nu_1-a_1), \\
&\max(0,\nu_1-(\iota+2-k-s)-a_1-b_1) \leqslant d_1 \\
&\leqslant \min(s,\nu_1-a_1-b_1)\big\}, \\
\bar{C}_\nu = \big\{&(r,s_1,g_1) \mid 1 \leqslant r \leqslant \iota-2,\ 0 \leqslant s_1 \leqslant \min(r,\nu_1), \\
&\max(0,\nu_1-1-s_1) \leqslant g_1 \leqslant \min(\iota-r-1,\nu_1-s_1)\big\}, \\
\bar{D}_\nu = \big\{&(r,m_1) \mid 0 \leqslant r \leqslant \iota,\ \max\big(0,\nu_1-(\iota-r)\big) \leqslant m_1 \leqslant \min(r,\nu_1)\big\}.
\end{aligned}$$

In these sets the index bounds are written in a consecutive manner so that they can be easily put into a program.

For $\bar{T}_\nu$ we obtain

$$\bar{T}_\nu = (1+c^2)^{-\iota/2} \sum_{t=0}^{\iota} \sum_{j_1=\max(0,\nu_1+t-\iota)}^{\min(t,\nu_1)} T_{(t,\iota-t)} \binom{t}{j_1} \binom{\iota-t}{\nu_1-j_1} (ic)^{t+\nu_1-2j_1}.$$

Step 2. *Computation of* $\bar{\phi}_\nu$, $|\nu| = \iota$.

Initially, for $\nu = (\iota, 0)$ we solve

$$\begin{bmatrix} J^{-1}(A-\lambda_{(\iota,0)}) & J^{-1}R \\ -R^T J^{-1} & 0 \end{bmatrix} \begin{bmatrix} \bar{\phi}_{(\iota,0)} \\ \varepsilon_{(\iota,0)} \end{bmatrix} = \begin{bmatrix} -J^{-1}\bar{T}_{(\iota,0)} \\ 0 \end{bmatrix}.$$

Then for $\nu = (\iota-1,1), (\iota-2,2), \ldots, (0,\iota)$ solve the linear system

$$D_\nu X_\nu = Z_\nu,$$

where

$$D_\nu = \begin{bmatrix} H_{uu}^0 - \lambda_\nu J^{-1} & J^{-1}R \\ -R^T J^{-1} & 0 \end{bmatrix}, \quad X_\nu = \begin{bmatrix} \phi_\nu \\ \varepsilon_\nu \end{bmatrix}, \quad \lambda_\nu = \sum_{j=1}^{2l} b_{j,j}\nu_j,$$

$$Z_\nu = \begin{bmatrix} J^{-1}((1+\nu_1)(1-c^2)\bar{\phi}_{(\nu_1+1,\nu_2-1)} - \bar{T}_\nu) \\ 0 \end{bmatrix}.$$

Step 3. *Computation of* $\phi_\nu, \psi_\nu, f_\nu, |\nu| = \iota$.

Recall

$$P^{-1} = P^\star = (1+c^2)^{-\iota/2} \begin{bmatrix} 1 & -ic \\ -ic & 1 \end{bmatrix},$$

which leads for ϕ_ι to the form

$$\phi_\iota(\omega) = \bar{\phi}_\iota(P^{-1}\omega) = (1+c^2)^{-\iota/2} \sum_{|\nu|=\iota} \bar{\phi}_\nu (\omega_1 - ic\omega_2)^{\nu_1} (\omega_2 - ic\omega_1)^{\nu_2}.$$

Therefore, the coefficients ϕ_ν of $\phi_\iota(\omega)$ are determined from

$$\phi_\nu = (1+c^2)^{-\iota/2} \sum_{t=0}^{\iota} \sum_{j_1=\max(0,\nu_1+t-\iota)}^{\min(\nu_1,t)} (-ic)^{t+\nu_1-2j_1} \binom{j_1}{t} \binom{\nu_1 - j_1}{\iota - t} \bar{\phi}_{(t,\iota-t)}.$$

When evaluating the equation

$$\psi_\iota = \frac{1}{2} J_l \sum_{r=1}^{\iota-2} \left(\psi_{r+1}'^T J_l \psi_{\iota-r} - \phi_{r+1}'^T J^{-1} \phi_{\iota-r}\right),$$

we obtain for the coefficients ψ_ν, $|\nu| = \iota$, the expression

$$\psi_\nu = \frac{1}{2} J_l \sum_{r=1}^{\iota-2} \sum_{t=\max(0,\nu_1-r)}^{\min(\iota-r,\nu_1)} \big(\psi_{(\nu_1-t,r+t-\nu_1)}'^T J_l \psi_{(t,\iota-r-t)} - \phi_{(\nu_1-t,r+t-\nu_1)}'^T J^{-1} \phi_{(t,\iota-r-t)}\big).$$

Here we use the derivatives of order $\iota - 1$.

For the order $|\nu| = \iota$ we obtain the following formulas:

$$\phi_\nu' = \phi_{(\nu_1+1,\nu_2)}(\nu_1+1)(1,0) + \phi_{(\nu_1,\nu_2+1)}(\nu_2+1)(0,1),$$
$$\psi_\nu' = \psi_{(\nu_1+1,\nu_2)}(\nu_1+1)(1,0) + \psi_{(\nu_1,\nu_2+1)}(\nu_2+1)(0,1).$$

Finally, we set $f_\nu = \phi_\nu + R\psi_\nu$, $f_\nu' = \phi_\nu' + R\psi_\nu'$.

Now repeat Step 1 with the next index ι.

We notice that in the course of the computations we can also derive approximations for the reduced Hamiltonian $M = H \circ f$ given by

$$M(\omega) = \frac{1}{2} f^T(\omega) H^{(2)}(0) f(\omega) + \frac{1}{n} \sum_{j=1}^{n-1} \big(f_{[j]}(\omega)\big)^3,$$

$$H^{(2)}(0) = \frac{1}{n} \operatorname{diag}\{-D, I_{n-1}\},$$

where $f_{[j]}(\omega)$ is the jth component of $f(\omega)$.

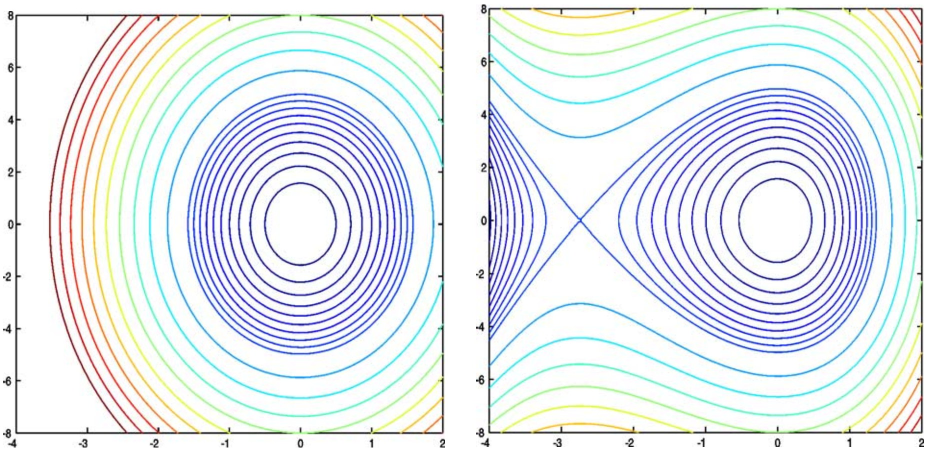

Fig. 1. Contour lines of M_2 and M_3 in $[-4,2]\times[-8,8]$ for $n=100$.

The approximations are $M_k(\omega)=\sum_{\iota=2}^{k} M_{\iota,d}(\omega)$, where $M_{\iota,d}(\omega)=\sum_{|\nu|=\iota} M_\nu\omega^\nu$ and

$$M_\nu=\frac{1}{n}\sum_{j=1}^{n-1}\sum_{(k,r,t,s)\in E_\nu} f_{[j](t,k-t)}\cdot f_{[j](s,r-s)}\cdot f_{[j](\nu_1-t-s,\iota-k-r-\nu_1+t+s)}$$
$$+\frac{1}{2}\sum_{j=1}^{\iota-1}\sum_{\max(0,j+\nu_1-\iota)}^{\min(j,\nu_1)} f_{(t,j-t)}^T H^{(2)}(0) f_{(\nu_1-t,\iota-j-\nu_1+t)},$$

where

$$E_\nu=\bigl\{(k,r,t,s)\mid 1\leqslant k\leqslant \iota-2,\ 1\leqslant r\leqslant \iota-1-k,$$
$$\max(0,\nu_1+k-\iota)\leqslant t\leqslant\min(k,\nu_1),$$
$$\max(0,\nu_1+k+r-\iota-t)\leqslant s\leqslant\min(r,\nu_1-t)\bigr\}.$$

This algorithm was implemented into a MATLAB code. In the case $n=100$ we obtained the following expression for M_5:

$$M_5(\omega_1,\omega_2)=4.9352\omega_1^2+0.5000\omega_2^2+1.2004\omega_1^3$$
$$+10^{-3}\bigl(3.6583\omega_1^4+0.1137\omega_1^2\omega_2^2-0.001278\omega_2^4\bigr)$$
$$+10^{-4}\bigl(2.1079\omega_1^5-0.05586\omega_1^3\omega_2^2+0.001017\omega_1\omega_2^4\bigr).$$

Here we set those coefficients to zero for which the numerical values were less than 10^{-15} in absolute value. The Hamiltonian of (4.3) has a $\mathbb{Z}_2$-symmetry $H(U,-V)=H(U,V)$ which is inherited by the approximate Hamiltonians as follows:

$$M_k(\omega_1,-\omega_2)=M_k(\omega_1,\omega_2).$$

Therefore, the coefficients involving odd powers of ω_2 must be equal to zero.

Figures 1 and 2 show the contour lines of M_2 and M_3 in a large window and a plot of the graphs of the differences M_4-M_3 and M_5-M_4 of the approximate Hamiltonian functions over the unit square.

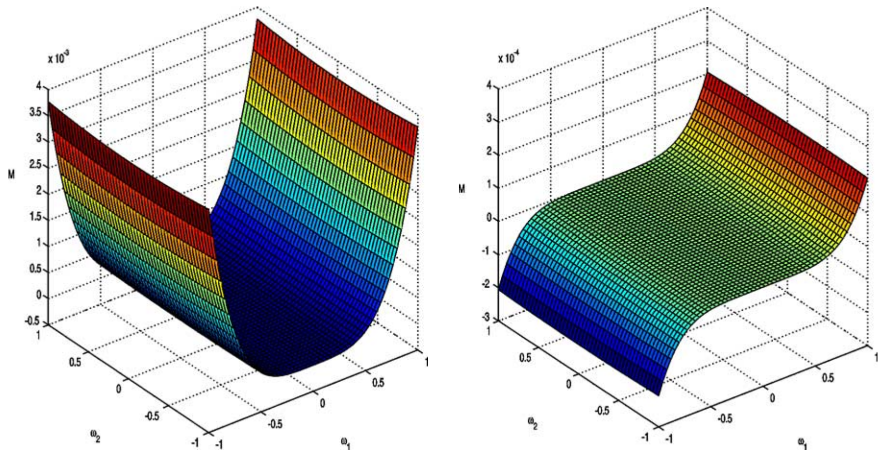

Fig. 2. $M_4 - M_3$ and $M_5 - M_4$ in $[-1,1] \times [-1,1]$ for $n = 100$.

Locally from M_2 to M_3 there is a big change in the contour plot while for M_4, M_5 the difference to M_3 is so small that is does not show up in the given window $[-4,2] \times [-8,8]$. Therefore we showed $M_4 - M_3$ and $M_5 - M_4$ in order to demonstrate convergence as $k \to \infty$.

Note also the scale 10^{-4} for the vertical axis in Fig. 2.

In this paper we have not analyzed the behavior of the center manifolds as $n \to \infty$. However, a formal comparison of the center manifold for the continuous system (4.1) and the discrete system (4.3) reveals that the function actually approximates the Hamiltonian function of the continuous case as $n \to \infty$.

For example, for the cubic term of M_3 a longer calculation yields the explicit expression (the cubic term of M_3 is a monomial)

$$c_n \omega_1^3 = \frac{1}{\sqrt{2}} \frac{1}{n} \left(3 \operatorname{ctg} \frac{\pi}{2n} - \operatorname{ctg} \frac{3\pi}{2n} \right) \omega_1^3.$$

For the coefficient one finds

$$c_n = \frac{8\sqrt{2}}{3\pi} + \frac{\pi^3}{15\sqrt{2} n^4} + O\left(\frac{1}{n^6}\right),$$

where

$$c_\infty \omega_1^3 = \frac{8\sqrt{2}}{3\pi} \omega_1^3$$

turns out to be the cubic term for the reduced Hamiltonian in the continuous case.

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